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## PART 4

### LM2-TOXIC

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#### Chapter 1. Executive Summary

As one of the components in the overall Lake Michigan Mass Balance Project (LMMBP) modeling framework, a comprehensive polychlorinated biphenyl (PCB) congener-based water quality model, LM2-Toxic, was developed to simulate fate and transport of PCBs in both water and sediment of Lake Michigan. The main focus of this model was to address the relationship between sources of toxic chemicals and their concentrations in water and sediments of Lake Michigan, and provide the PCB exposure concentrations to the bioaccumulation model (LM2 Food Chain) to predict PCB concentrations in lake trout tissue. This report provides detailed model description and development, model input and field data, model calibration procedures and confirmation, PCB mass budget analysis, the results of model predictions, and sensitivity analyses.

LM2-Toxic is a revision of the United States Environmental Protection Agency (USEPA)-supported WASP4 water quality modeling framework. It incorporates the organic carbon dynamics featured in GBTOX and the sediment transport scheme, a quasi-Lagrangian framework, used in the IPX. Both GBTOX and IPX were WASP4-type models and major components in the Green Bay Mass Balance

Project (GBMBP) modeling framework. Another important modification was the addition of updated air-water exchange formulations to the model.

There were 94 segments in the spatial segmentation for the LM2-Toxic. Forty-one of them were water column segments, and 53 of them were surficial sediment segments. Temporal resolution for the model input was on a daily time scale. Most of the kinetic functions were segment-specific time functions. Good representation of water circulation was essential for the accuracy of outputs from the water quality model. The results at 5 x 5 km<sup>2</sup> grid generated by Princeton Ocean Model (POM) for the Great Lakes were linked to the transport fields for LM2-Toxic. Due to an affinity of PCBs for organic carbon, three organic carbon sorbents were simulated as state variables in LM2-Toxic. They were biotic carbon (BIC), particulate detrital carbon (PDC), and dissolved organic carbon (DOC). The model simulated 54 PCB congeners which accounted for roughly 70% of the total PCB mass in Lake Michigan. Four phases were simulated in LM2-Toxic for the congeners. The four phases were dissolved, sorbed to PDC, sorbed to BIC, and bound to DOC.

LM2-Toxic is a coupled mass balance of organic carbon solids and toxic chemical (PCBs) dynamics. Prior to the organic carbon dynamics and PCB

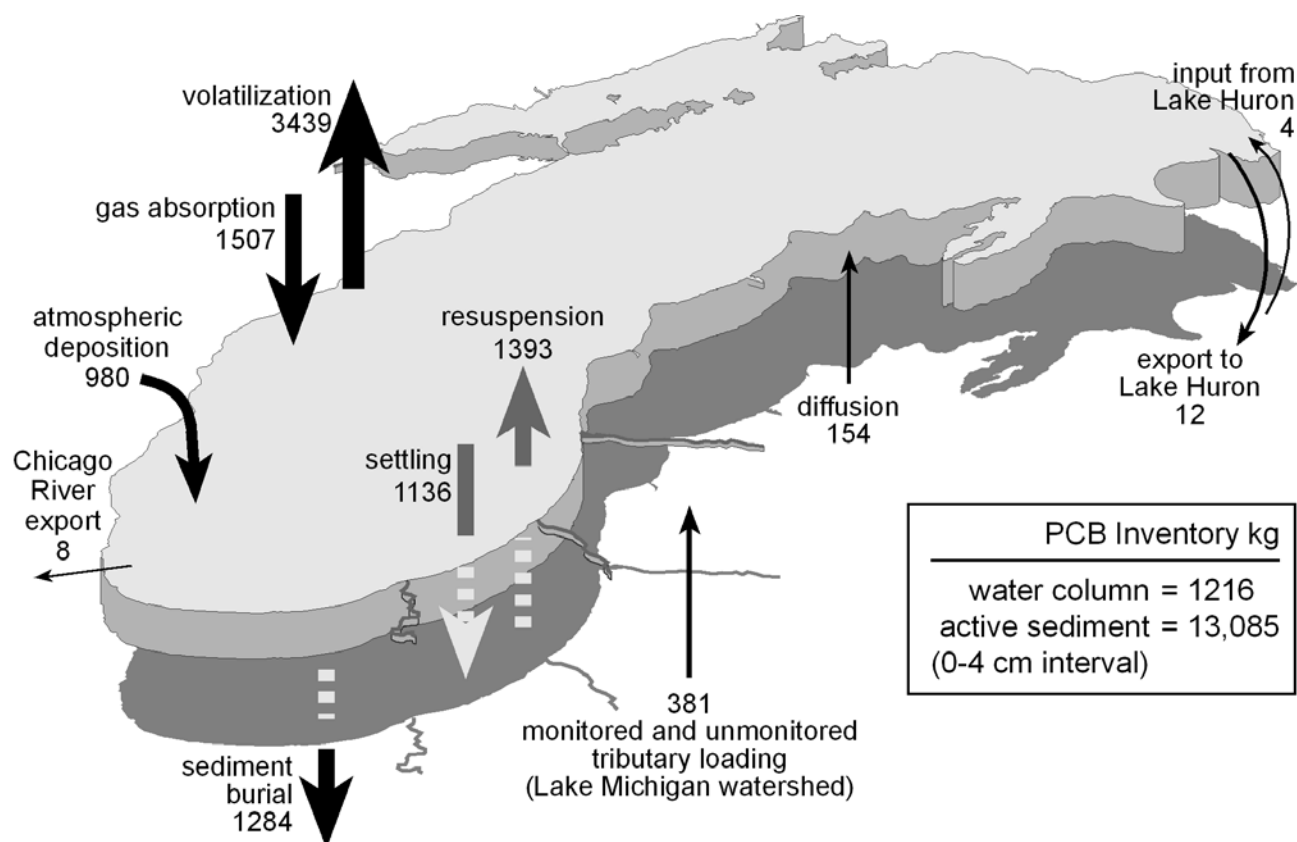
dynamic calibrations, vertical dispersion coefficients were determined using a thermal balance model. Using the LMMBP-generated field data, the organic carbon solids dynamics were first calibrated. This was followed by the independent calibration of PCB dynamics. The temporal variations of both BIC and PDC resulted from an algal bloom in late spring and early summer. Primary production was the dominant organic carbon load to Lake Michigan. The eutrophication model (LM3-Eutro)-generated primary production accounted for over 90 percent of the total particulate organic carbon (POC) load to the lake. The PCB concentrations in the dissolved phase was about double the concentration in the particulate phase in the main lake. There was some degree of temporal variation in the water column PCB concentration controlled by a combination of seasonal variation of external loads, atmospheric concentrations, and sediment resuspension events. There was also a slight longitudinal concentration gradient throughout the main lake. The highest concentrations were found in the southern segments due to higher PCB atmospheric deposition and concentrations observed in the area close to Chicago. There was little vertical gradient of PCB concentrations found based on main lake cruise mean data. As an important part of the modeling effort to reduce uncertainties associated with water transport, settling, resuspension, and sedimentation, a chloride model, a long-term simulation using a  $^{137}\text{Cs}$  and  $^{239,240}\text{Pu}$  model, a long-term organic carbon simulation, and a 47-year PCB hindcast simulation using LM2-Toxic were developed and run for LM2-Toxic confirmation. These confirmation steps were crucial and laid down a credible foundation for long-term projections using LM2-Toxic.

After calibration of organic carbon and PCB congener dynamics and model confirmation, a mass budget analysis was done for the LMMBP period (1994-1995) to identify the critical contaminant sources, sinks, and key environmental processes in Lake Michigan. Figure 4.1.1 provides a summary of the results of the total PCB mass budget diagnosis in Lake Michigan. The average masses of total PCBs presented in the water column and the surficial sediments (0-1 cm) of the lake during 1994-1995 were 1,216 kg and 13,085 kg, respectively. The inventories divided by the volumes of the water and the surficial sediment layer of the lake lead to an average concentration of total PCBs equal to 0.259

ng/L in the water column and 12,037 ng/L in the surficial sediment layer. The information on the fluxes of total PCBs in Figure 4.1.1 shows the single largest flux leaving the Lake Michigan system was gross volatilization. This flux was countered by the flux from gas absorption as the largest source to the lake. The air-water exchange was the most important process for Lake Michigan. It produced the largest PCB net loss out from the lake. Resuspension was a major influx of PCBs to the water column offset by the flux from settling. Resuspension and settling were very important processes in the lake system. The results of these processes made the net flux between resuspension and settling the second largest net source. The total external load (tributary loads + atmospheric loads) to the water column of the lake was the largest net PCB source to the lake water column. The flux by burial was the largest net loss from the surficial sediment layer. There was a net loss of 1,863 kg/year of total PCBs for the entire Lake Michigan system (the water column + the surficial sediment layer of both Green Bay and Lake Michigan). This indicated both the water column and the surficial sediment layer of the lake were not at steady-state during the LMMBP period.

The model was also applied for forecasting the long-term responses (62-year simulation, starting on January 1, 1994) of the PCBs in Lake Michigan under various forcing functions and load reduction scenarios. Seven PCB forecast and sensitivity scenarios were conducted. These seven long-term forecast and sensitivity scenarios were:

- A. Constant Conditions (Upper Bound) – Repeat 1994-1995 conditions.
- B. Continued Recovery (Fast) – Atmospheric components (vapor phase concentration, dry and wet depositions) decline with a six-year half-life (Hillery *et al.*, 1997; Schneider *et al.*, 2001). Tributary loads decline with a 13-year half-life (Endicott, 2005; Marti and Armstrong, 1990).
- C. Continued Recovery (Slow) – Atmospheric components (vapor phase concentration, dry and wet depositions) decline with a 20-year half-life (Buehler *et al.*, 2002). Tributary loads decline with a 13-year half-life.

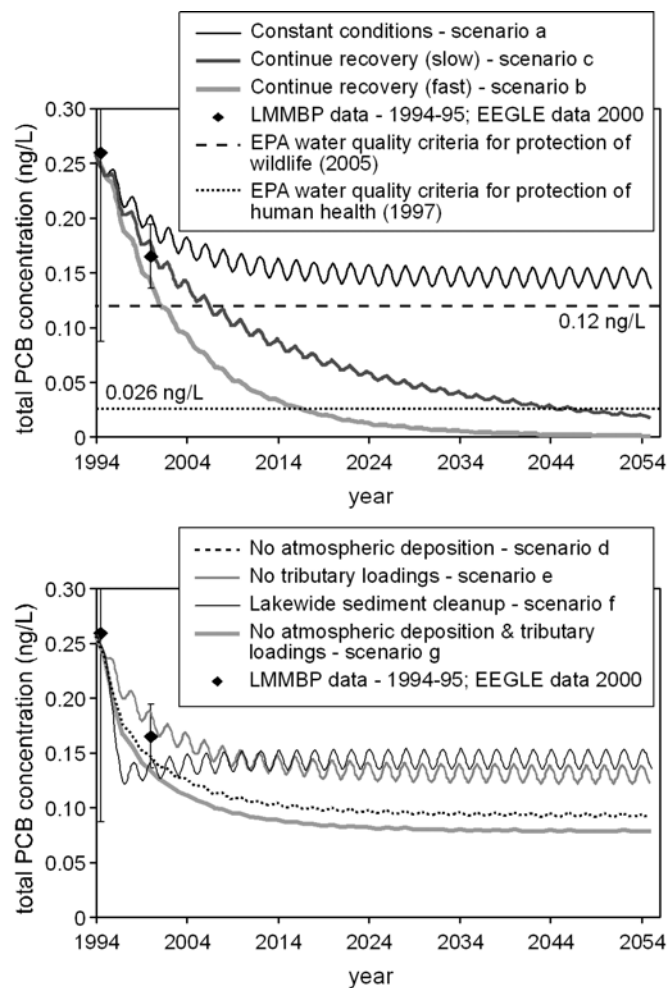


**Figure 4.1.1. Mass budget average for 1994-1995 total PCBs in the Lake Michigan system (including Green Bay). Unit of the masses transported (arrows) is in kg/year.**

- D. No Atmospheric Deposition – Stop all PCB atmospheric deposition (dry and wet).
- E. No Tributary Loadings – Stop all tributary PCB loads.
- F. Lake Sediment Clean-up – Remove all PCB mass from the surficial sediments.
- G. No Atmospheric Deposition and No Tributary Loadings – Stop all PCB atmospheric deposition (dry and wet) and tributary loads.

All of the control actions started on January 1, 1996. Figure 4.1.2 presents the long-term responses of total PCBs in the water column of Lake Michigan under the seven forecast and sensitivity scenarios. The results from the Constant Conditions Scenario simulation clearly demonstrated that, during the

LMMBP period, the Lake Michigan system was not at steady-state with respect to the 1994-1995 loads, vapor phase concentrations, and the level of sediment total PCB inventory. The results from this scenario also indicate that, if there is no decline in the current (1994-1995) forcing conditions, the water column PCB concentration in the future will never meet the USEPA water quality criteria for the protection of wildlife (0.12 ng/L) (U.S. Environmental Protection Agency, 2005) and human health (0.026 ng/L) (U.S. Environmental Protection Agency, 1997) in the Lake Michigan system. The long-term response from Scenario B – Continue Recovery (Fast) shows that it takes about five years for the water column concentration to reach the USEPA water quality criterion for the protection of wildlife and more than two decades to reach the USEPA water quality criterion for the protection of human health. The water column PCB concentrations predicted in



**Figure 4.1.2. Annual long-term responses of total PCB concentrations in the water column of Lake Michigan for the forecast and sensitivity scenarios.**

Scenario C – Continue Recovery (Slow) declined at a much slower pace. The model results indicated that it takes about 12 years for the water column PCB concentrations in the lake to reach the USEPA water quality criterion for the protection of wildlife and that the water column PCB concentration will reach the USEPA water quality criterion for the protection of human health around 2046 (five decades after 1996). The rates used in Scenarios B and C may not be realistic rates for the Great Lakes in the future. With the addition of more recent data, it appears that the rate of decline in the atmospheric components could be slower than the decline rate used in Scenario C.

The results from the sensitivity scenarios (Scenarios D, E, F, and G) suggested that the long-term PCB

concentrations in the water column are more sensitive to atmospheric deposition (dry and wet) than to tributary loads. By eliminating PCB total inventory in the lake sediments on January 1, 1996, the water column concentration had a steep drop initially, and then gradually increased and reached a value close to the steady-state concentration predicted by Scenario A – Constant Condition.

LM2-Toxic is a sophisticated and state-of-the-art toxic chemical fate and transport model for Lake Michigan. There are still many improvements that can be made to the modeling framework and more systematic tests could be conducted to address the impacts of each process conceptualized in the LM2-Toxic on the model outcomes. The results and

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predictions from the LM2-Toxic clearly demonstrate the ability of the model to quantitatively analyze the behavior of PCBs in the Lake Michigan system and to forecast the long-term PCB dynamics under various external forcing conditions.

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